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A Parametric Transformation at Numerical Integration of ODE

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Abstract. The initial value problem for ordinary differential equation (ODE) is investigated when the linear parametric transformation (rotation of coordinate axes) is applied. It is shown that for transformed equation the principal term of asymptotic error expansion of numerical method can be minimized by an angle of rotation. The dependence of the optimal angle $\phi_{opt}(\lambda)$ on λ is plotted for the model equation $\frac{dy}{dx} = \lambda y$ solved by linear multistep methods and Runge-Kutta methods.

We study the numerical integration of ordinary differential equation of the form

$$\frac{dy}{dx} = f(x, y), \quad a \le x \le b, \quad y(a) = y_0. \tag{1}$$

Before solving this problem with one of the standard numerical methods we will try to transform Equation (1) into one that can be easy. Usually either new variables are introduced or a problem with known analytical solution is used. One such approach to the numerical solution of ODE is that of [1] which considers the integration of systems of the form $y'(x) = A(x)\, y + \epsilon f(x, y)$ with "small" $\epsilon > 0$. Thus we seek some transformation, simplifying the process of solution of a given problem. For example, when $f(x, y) = 1 + y^2$, the integration curve has points of infinite gradient at $x = \pm n\pi/2$. This curve can be found more simply if we transform Equation (1) into new coordinates (t, u) by the rotation of axes, as shown in Figure 1.

Note that the standard methods for the integration of ODE are usually based on algorithms adapting to a given problem (in the sense of automatical selection of a stepsize, order of a method, etc.). On the contrary, in our case we will adapt a problem to a given algorithm. There has been little theoretical investigation of such approach. Certainly the choice of appropriate transformation is art rather than algorithm. That is one of reasons that the "transformation" approach is not widely used. However, we can look for a family of transformations with some free parameters and try to simplify the choice by parameter optimization.

In this paper we consider the linear parametric transformation consisting in the rotation of coordinate axes where the angle of rotation is a parameter. The same transformation has formerly been used for regularization of the boundary value problem for ODE [2].

Let us introduce the new variables

$$u = x \cos\phi + y \sin\phi, \quad t = -x \sin\phi + y \cos\phi.$$

Then (1) can be transformed into

$$\frac{du}{dt} = g(t, u, \phi), \quad \alpha \le t \le \beta, \quad u(\alpha) = u_0, \tag{2}$$

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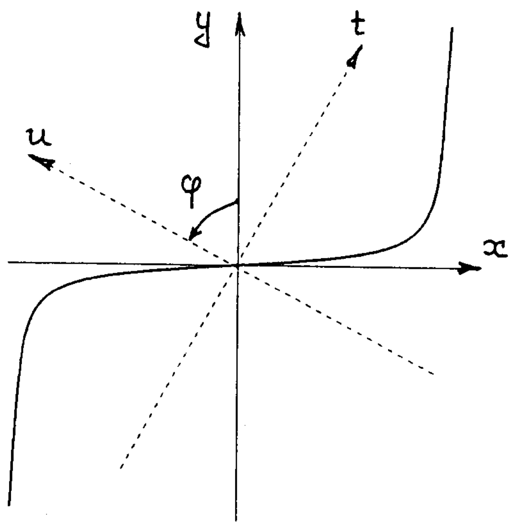

Figure 1.

where $\alpha = a\cos\phi + y_0 \sin\phi$, $\beta = b\cos\phi + y(b)\sin\phi$, and

$$g(t,u,\phi) = \frac{f(x,y)\cos\phi - \sin\phi}{f(x,y)\sin\phi + \cos\phi}.$$

It is assumed that $f\sin\phi + \cos\phi \neq 0$ for all t, ϕ.

Now the function $g(t,u,\phi)$ depends on a parameter ϕ—the angle of axes rotation. This result allows us to handle the right-hand side function and its partial derivatives by the rotation angle in order to minimize the error of numerical method. The asymptotic expansion of the global absolute truncation error when solving problem (1) is [3]

$$\epsilon_k = CH^s \int_{x_0}^{x_k} \exp\left[\int_{\xi}^{x_k} \frac{\partial f(\eta, y, (\eta))}{\partial y}\, d\eta\right] D_s\left[f\left(\xi, y(\xi)\right)\right] \nu^s(\xi)\, d\xi + O(H^{s+1}),$$

where s, order of the method; C, the error constant; $D_s[f(x,y)]$, certain differential operator associated with the method; $\nu(x)$, stepsize distribution function for irregular grid; and H, parameter of the grid. Obviously we also can write such an expansion for problem (2), but the error ϵ_k will depend on ϕ in this case. Therefore, it can be possible to minimize the error $\epsilon_k(\phi)$ by choosing an appropriate rotation angle.

The conventional numerical methods are based on local approximation of the solution by a polynomial and usually evaluate the local truncation error in order to select a suitable stepsize. The method is to estimate the principal term of asymptotic expansion of the local truncation error

$$R_s(h) = Ch^{s+1} D_s[g(t_k, u(t_k), \phi)] \tag{3}$$

and to select a stepsize h as large as possible which provides norm of $R_s(h)$ smaller than given tolerance τ. Let us introduce the "max" norm $\|\cdot\|_C = \max|\cdot|$ in the interval $[\alpha,\beta]$. Therefore, it would be interesting to consider the following minimization problem:

$$\min_{\phi} \max_{\alpha\le t\le\beta} \mid D_s[g(t,u(t),\phi)] \mid. \tag{4}$$

With a linear multistep method of order s, the differential operator is $D_s[g(t,u,\phi)] = g^{(s)}(t,u,\phi)$. Other methods, such as Runge-Kutta methods, have operators that involve partial derivatives of the right-hand side function.

EXAMPLE: Consider the model equation

$$\frac{dy}{dx} = \lambda y, \quad \lambda = \text{const},\ x \in [0,1],\ y(0) = 1 \tag{5}$$

which is transformed into

$$\frac{du}{dt} = \frac{\lambda(t\sin\phi + u\cos\phi)\cos\phi - \sin\phi}{\lambda(t\sin\phi + u\cos\phi)\sin\phi + \cos\phi}, \tag{6}$$

and solved by the Euler method with the following operator

$$D_1\left[g(t,u(t),\phi)\right] = g^{(1)}(t,u,\phi) = \frac{\lambda^2(t\sin\phi + u\cos\phi)}{\left(\lambda(t\sin\phi + u\cos\phi)\sin\phi + \cos\phi\right)^3}.$$

Returning to the old variables we receive the minimization problem

$$\min_{\phi}\ \max_{0\le x\le 1}\left|\frac{\lambda^2 y(x)}{\left(\lambda y(x)\sin\phi + \cos\phi\right)^3}\right|, \tag{7}$$

where $y(x) = y_0\exp(\lambda x)$ is the known solution. Further, let $y^*(\phi)$ be a value of y (depending on ϕ), which provides the maximum of $D_1[g]$ with respect to x. Observing that the expression under modulus sign is positive at $\lambda y_0 \sin\phi \ge 0$, we can use the necessary condition of the extremum $\frac{\partial\| D_1[g]\|_C}{\partial y} = 0$ and find

$$y^*(\phi) = \begin{cases} y_0, & \text{if } \mathrm{ctg}(\phi) > 2\lambda y_0,\\ y_0\exp(\lambda), & \text{if } \mathrm{ctg}(\phi) < 2\lambda y_0\exp(\lambda),\\ \frac{1}{2\lambda}\mathrm{ctg}(\phi), & \text{elsewhere.}\end{cases}$$

In order to obtain the optimal value ϕ_{opt} we use another necessary condition $\frac{\partial\| D_1[g]\|_C}{\partial\phi} = 0$, assuming that $y^*(\phi) = (1/2\lambda)\mathrm{ctg}(\phi)$. We thus obtain the optimal value

$$\phi_{opt} = \pm\arccos\sqrt{\frac{2}{3}} \quad \text{if } 2\lambda y_0 \le \mathrm{ctg}(\phi_{opt}) \le 2\lambda y_0\exp(\lambda), \tag{8}$$

where sign of ϕ_{opt} is determined from the condition $\lambda y_0\sin\phi \ge 0$. It is worth remarking that the maximum of $D_1[g]$ at optimal angle ϕ_{opt} about λ times less than one at $\phi = 0$.

Let us consider further the Runge-Kutta methods (RKMs) presented by the Butcher table of coefficients a_{ij}, b_i, c_i defining the method [4]. In case of second order method, the principal term of asymptotic expansion of the local error can be written in the form

$$R_2(h) = \frac{h^3}{3!}\left[g^{(2)} - 3b_2c_2^2(g_{tt} + 2gg_{tu} + g^2g_{uu})\right].$$

By regarding $g(t,u,\phi)$ as function of x and $y(x)$ we derive

$$g^{(1)} = \frac{f^{(1)}}{(f\sin\phi + \cos\phi)^3}, \quad g^{(2)} = \frac{f^{(2)}(f\sin\phi + \cos\phi) - 3(f^{(1)})^2\sin\phi}{(f\sin\phi + \cos\phi)^5}, \quad \text{etc.}$$

Then we can obtain following expression for the principal term when solving the model problem

$$R_2(h) = \frac{h^3}{3!}\,\frac{\lambda^3 y(x)\cos\phi - 2\gamma\lambda^4y^2(x)\sin\phi}{(\lambda y(x)\sin\phi + \cos\phi)^5}, \quad y(x) = y_0\exp(\lambda x). \tag{9}$$

Here $\gamma = 1 - 3b_2c_2^2$ is the method-depended constant. As far as the method of third order is concerned, we have

$$\begin{aligned}R_3(h) = \frac{h^4}{4!}&\left[g^{(3)} - 4(b_2c_2^3 + b_3c_3^3)\,(g_{ttt} + 3gg_{ttu} + 3g^2g_{tuu} + g^3g_{uuu})\right.\\ &-\left. 4c_3(g_tg_{tu} + gg_ug_{tu} + gg_tg_{uu} + g^2g_ug_{uu}) - 2c_2(g_{tt}g_u + 2gg_ug_{tu} + g^2g_ug_{uu})\right].\end{aligned}$$

Returning to the old variables we receive for the model equation

$$R_3(h) = \frac{h^4}{4!} \frac{6\gamma\lambda^6 y^3(x)\sin^2\phi + 4\omega\lambda^5 y^2(x)\sin\phi\cos\phi + \lambda^4 y(x)\cos^2\phi}{(\lambda y(x)\sin\phi + cos\phi)^7}. \tag{10}$$

Here $\gamma = 1 - 4(b_2c_2^3 + b_3c_3^3)$, $\omega = c_2 + 2c_3 - 2$. Note that for linear multistep methods (LMMs) of the second and the third orders $\gamma = 1$, $\omega = -2$.

Let us now turn to the minimization problem of the local error in the L_2-norm $\|\cdot\|_{L_2}$. In this case we have following problem (in the old variables)

$$\min_{\phi} \int_0^1 D_s^2\left[g\left(x, y(x), \phi\right)\right]\ \left(y'(x)\sin\phi + \cos\phi\right)\, dx. \tag{11}$$

Then we obtain for the Euler method when solving the model equation (5)

$$\min_{\phi} \int_0^1 \frac{\lambda^4 y_0^2 \exp^2(\lambda x)}{(\lambda y_0 \exp(\lambda x)\sin\phi + \cos\phi)^5}\, dx.$$

We are also able to write such problems for the methods of orders 2 and 3 by change of differential operator in (11). These problems have been solved for $\lambda \in [-100, -1]$ and the dependences $\phi_{opt}(\lambda)$, providing $\min \|\, D_s[g]\, \|_{L_2}$.

First, we examine linear multistep methods. Figure 2 shows the plots $\phi_{opt}(\lambda)$ for the Euler method (curve 1), LMM of the second order (curve 2) and LMM of the third order (curve 3). Further, plots for some RKMs of order 2 are shown in Figure 3, namely, the trapezoidal method (curve 1) with $c_2 = 1$ (i.e. $\gamma = -1/2$), classical Runge method (curve 2) with $c_2 = 1/2$ (i.e., $\gamma = 1/4$) and the method with $c_2 = 2/3$, $\gamma = 0$ (curve 3). At last, Figure 4 shows plots for third order RKMs: the Runge method (curve 1) with $c_2 = 1/2$, $c_3 = 1$ ($\gamma = 0, \omega = 1/2$), the Heun method (curve 2) with $c_2 = 1/3$, $c_3 = 2/3$ ($\gamma = 1/9, \omega = -1/3$) and the method with $c_2 = 1/2$, $c_3 = 3/4$, $\gamma = 1/12$, $\omega = 0$ (curve 3). All of the dependences are plotted in the logarithmic scale, and values of ϕ are given in radians. It is interesting that $\phi_{opt}(\lambda)$ has different asymptotic behavior for the third order Runge-Kutta methods, but not so when the order is 2.

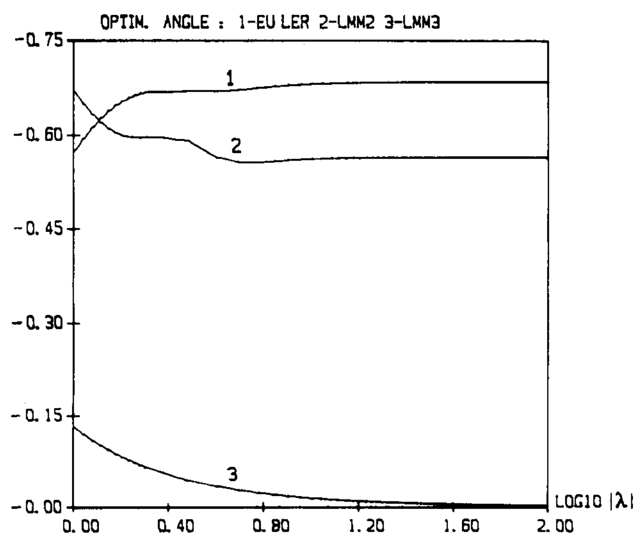

Figure 2.

Finally we shall briefly discuss the results. Preliminary transformation of the initial problem allows us to minimize the principal term of asymptotic error expansion in some norm by parameter optimization. Therefore, we are able to solve the transformed equation

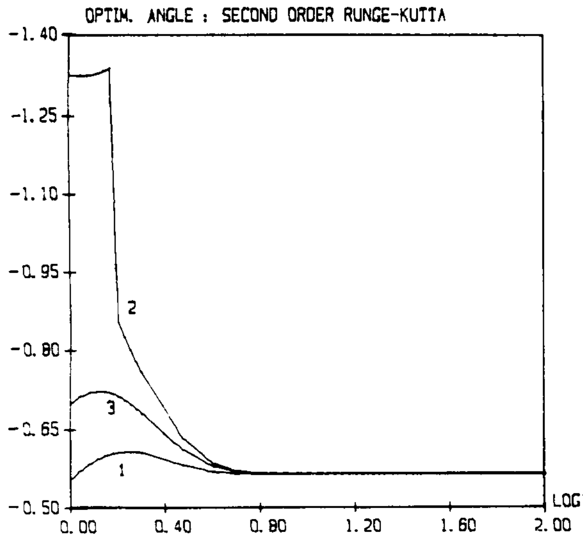

Figure 3.

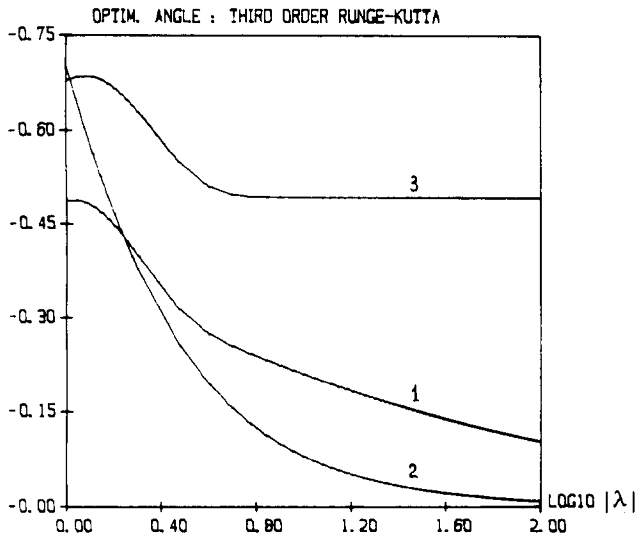

Figure 4.

more efficiently with standard methods as a consequence of possible stepsize extension or decreasing the method order. Note that this transformation can also be used with another methods, such as Picard iterations, and so on. It must be pointed out that our results hold true when there is no need to present the solution in the old coordinates. If we return to the old coordinates, the errors of the nodes, x_k, will arise due to the involvement of both dependent and independent variables in the rotation. In this case the full error will be determined by the formula

$$|y(x_k) - y_k| \approx \epsilon_k(\cos\phi - f(x^*, y(x^*))\sin\phi),$$

where $x^* = x_k + \theta(x_{k+1} - x_k)$, $0 \le \theta \le 1$, $\epsilon_k = |u(t_k) - u_k|$, $y(x_k), u(t_k)$ are exact solutions of the problems (1) and (2) and y_k, u_k are appropriate numerical solutions. It has to be admitted that the "rotation" approach does not seem to be efficient when presenting the solution in the old coordinates.

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